

Energy Ambiguity in Nonlinear Quantum Mechanics

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Abstract

We observe that in nonlinear quantum mechanics, unlike in the linear theory, there exists, in general, a difference between the energy functional defined within the Lagrangian formulation as an appropriate conserved component of the canonical energy-momentum tensor and the energy functional defined as the expectation value of the corresponding nonlinear Hamiltonian operator. Some examples of such ambiguity are presented for a particularly simple model and some known modifications. However, we point out that there exist a class of nonlinear modifications of the Schrödinger equation where this difference does not occur, which makes them more consistent in a manner similar to that of the linear Schrödinger equation. It is found that necessary but not sufficient a condition for such modifications is the homogeneity of the modified Schrödinger equation or its underlying Lagrangian density which is assumed to be “bilinear” in the wave function in some rather general sense. Yet, it is only for a particular form of this density that the ambiguity in question does not arise. A salient feature of this form is the presence of phase functionals. The present paper thus introduces a new class of modifications characterized by this desirable and rare property.

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1 Introduction

Nonlinear equations are widespread in physics. Some of them have a fundamental status, to name Einstein's equations in general relativity or nonlinear equations of non-Abelian gauge theories. On the other hand, there is a good deal of nonlinear equations that are a result of some natural physical approximations induced by particular conditions, such as, for instance, caused by a nonlinear response of a medium to propagation of a signal whose motion is otherwise governed by linear equations [1, 2, 3].

In view of the ubiquity of nonlinear equations in physics and the singular importance of the Schrödinger equation (SE), it is not completely untenable to conceive that the linear Schrödinger equation is an approximation to a more fundamental nonlinear equation. No strong evidence to the contrary has been provided yet. Meanwhile, this hypothesis has motivated many authors to either explore fundamental premises that the basic equation of quantum mechanics might, or even ought to be, nonlinear, sometimes along with more or less general proposals of accomplishing this in a consistent manner, or to invent arguments against this case on a fundamental level. What has indeed been observed is that in some circumstances this equation naturally acquires a nonlinear extension, typically in a description of phenomena involving many particles, to name one but exquisitely important an instance, the Bose-Einstein condensate. In this case, the leading correction in the mean-field approach to this system results in the cubic nonlinear Schrödinger equation which in the context under discussion is often referred to as the Gross-Pitaevskii equation [4, 5, 6]. Therefore, even if the Schrödinger equation may never be found truly nonlinear, the quantum mechanical picture of reality can equally well be found incomplete without nonlinearities aimed to describe particular physical effects phenomenologically. As a result of these two approaches, fundamental and phenomenological, a large and growing literature originating from different philosophies has been devoted to nonlinear modifications of quantum mechanics, and, in particular, modifications of its fundamental equation.

A consistent theoretical framework for nonlinear quantum mechanics (NLQM) was given by Mielnik [7] who also pointed out [8] that since there exist many different probability models, they may be related to some nonlinear variants of quantum mechanics. Even though nonlinear extensions of the Schrödinger equation are usually assumed to depart from its linear counterpart in some reasonably small way, certain qualitatively new changes can occur. This is, for instance, demonstrated by the mobility phenomenon [9, 10] reflecting the fact that the scalar product is not conserved for quantum states whose evolution is governed by a nonlinear equation. Two basic and physically important properties of the standard Schrödinger equation are, as a rule, sacrificed in NLQM. One is the linear superposition principle that can never¹ be maintained while the other is the separability of composite systems that can be preserved in some nonlinear modifications of this equation. It is the latter property that has acquired a privileged status for it can discriminate between more and less physically tenable modifications. Indeed, the lack of separability leads to rather unacceptable physical consequences: even in the absence of any interactions the motion of one wave packet can affect the behavior of the other one in a composite system consisting of these two packets, which clearly violates causality. In its original form [12], this condition required that a physically acceptable nonlinearity should allow two separated, noninteracting and noncorrelated subsystems to evolve independently of each other. The essential element of this postulate is that the subsystems are uncorrelated, meaning that the total wave function is the product of composite wave functions. Equations that have such a separability property have come to be called weakly separable [21]. As shown in [13], this property naturally occurs in a class of nonlinear Schrödinger equations characterized by a certain homogeneity property. The

¹In some rare cases [38, 39] it can be partially retained, though.

equations of this class which include those proposed by Kostin [11], Białynicki-Birula and Mycielski [12], and Doebner and Goldin [32, 33] are related via generalized nonlinear gauge transformations [34]. Nevertheless, it was noted [14, 15, 16, 17] that weakly separable equations may still violate causality if the initial state of a composite system is entangled.

On the other hand, it was found [18, 19, 20] that there exists a class of deterministic, i.e. non-stochastic, nonlinear generalizations of quantum mechanics in which the mentioned causality problems can be avoided for both pure-entangled and general-mixed states if an appropriate multi-particle extension is used. Such modifications can be called strongly separable [21]. Based on this observation, a novel general approach to the issue of separability has recently been put forward by Czachor [21]. This approach chooses as its starting point the nonlinear von Neumann equation for the density matrices [22] and proceeds from there to the n -particle extension. In a sense, one can call this approach “effective” as opposed to the “fundamentalist” one. The latter approach does not resort to reformulating in terms of density matrices various proposed in the literature nonlinear modifications of the Schrödinger equation that, similarly as the linear equation itself, are postulated to be obeyed by pure states. The problem of nonlocality is confounded since these approaches, even though they belong to the same strong separability framework, yield different results. For instance, the Białynicki-Birula and Mycielski modification that is weakly separable and strongly in the effective approach turns out to be essentially nonlocal in the fundamentalist approach for a general nonfactorizable two-particle wave function as recently demonstrated by Lücke [23]. The same applies to the Doebner-Goldin modification that being both weakly and strongly separable in the effective approach fails to maintain the separability for a more general nonfactorizable wave function describing a system of two particles if the fundamentalist approach is used. Only in some special case, that corresponds to the linearizable Doebner-Goldin equation, are the particles separable in the latter approach [24].

The work of Weinberg [14, 25], that proposed a relatively general framework for possible nonlinear modifications of quantum mechanics, has renewed and greatly stimulated the interest in various aspects of nonlinear quantum mechanics and, in particular, in modifications of the fundamental equation of this theory. It is in Weinberg’s framework that the homogeneity property, adopted from the linear Schrödinger equation, becomes elevated to one of the fundamental assumptions of nonlinear generalization of quantum mechanics. Although already present in some earlier modifications of this equation [26, 27, 28, 29], the authors of the proposals following Weinberg’s [30, 31, 32, 33, 35, 36, 37, 38, 39] have also considered this property an essential feature of their modified Schrödinger equation. The main general motivation to retain this feature in the generalized nonlinear framework is to ensure that the departure from the linear structure of quantum mechanics is not as dramatic as to render the modified scheme loose all relevant properties of this theory. The basic physical consequence of preserving this property in a nonlinear version of the Schrödinger equation is that, similarly as in linear theory, any two wave functions Ψ and $\lambda\Psi$ represent the same physical state. Weinberg also noted that the homogeneity is sufficient to guarantee the weak separability of composite systems. However, even if this is true in his modification and in some others that possess the property in question [13, 27, 35, 38, 39], it cannot be generically extended as shown by some example of homogeneous yet nonseparable nonlinear Schrödinger equation [37]. It has also been demonstrated [21] that the homogeneity is not in the least necessary for the strong separability of nonlinear variants of this equation in the effective approach. Therefore, it seems that, in principle, there is no compelling reason to require it in the general nonlinear theory. In the light of these arguments, it is not completely unfounded to conceive that the property in question is probably an accidental feature of the discussed equation and thus disposing of it in a nonlinear scheme may not necessarily cause a tremendous

departure from the linear structure of the theory. It is the main purpose of this paper to demonstrate that this is not the case as indeed eliminating this property does entail rather dramatic consequences. As we will see, compromising homogeneity leads to an ambiguity in the expression for the energy of a quantum-mechanical system that in the case of the linear Schrödinger equation is uniquely determined both as the expectation value of a Hamiltonian that serves as the generator of evolution and in the field-theoretical Lagrangian framework as a constant of motion for systems whose Lagrangian does not depend explicitly on time. In nonlinear theory, the discussed property is in general sacrificed, meaning that these two objects represent different quantities. It is the main purpose of this paper to show that there exists a class of nonlinear modifications of the fundamental equation of quantum theory that preserve the property in question and to spell out the conditions under which this occurs.

To this end, in the next section we present the ambiguity in its general form and point out that there exist a well-defined class of nonlinear modifications of the Schrödinger equation in which it does not arise. The examples of modifications affected by the problem in question are discussed in the section that follows as are the examples of the modifications already put forward in the literature in which the ambiguity is absent. Our findings are summarized in the conclusions. The appendix contains a more detailed presentation of how we arrived at the class of ambiguity-free modifications.

2 Ambiguity

In what follows, we will consider nonlinear modifications of the Schrödinger equation that possess a Lagrangian formulation. Consequently, as just noted, as long as the Lagrangian is not explicitly time-dependent (that is, for instance, the potentials in which quantum-mechanical systems evolve are time-independent), the energy of such systems can in principle be a conserved quantity. The quantity in question is defined as a space integral over the time-time component of the corresponding canonical energy-momentum tensor. This energy functional, that we choose to call field-theoretical, can then be contrasted with the energy functional which we term quantum-mechanical for it is defined as an expectation value of the Hamiltonian operator H . In NLQM, as we will see, once the Lagrangian for a modification is defined, one finds this operator from its equations of motion. In linear quantum mechanics these two definitions of energy coincide.

We will deal only with wave functions that are square-integrable and thus normalizable in the norm naturally induced by the scalar product

$$\langle \Psi_1 | \Psi_2 \rangle \equiv \int d^3x \Psi_1^*(\vec{x}) \Psi_2(\vec{x}). \quad (1)$$

Let us denote the total Lagrangian density for a modified Schrödinger equation by $L(R, S)$ and its Hamiltonian operator by $H(R, S)$, where R and S stand for the amplitude and the phase of the wave function, $\Psi = R \exp(iS)$, correspondingly. Now, $L(R, S) = L_{SE}(R, S) - L_{NL}(R, S)$ and $H(R, S) = H_{SE}(R, S) + H_{NL}(R, S)$, where subscripts SE and NL denote the parts leading to or corresponding to a purely linear and a nonlinear “correction” of these quantities, respectively. We will use this hydrodynamic representation [40] throughout the rest of the paper. We assume that the Lagrangian density does not contain differential position operators of the order higher than second and time derivative terms beyond those that appear in its linear part. The former assumption is made solely for the sake of simplifying our considerations. We also assume that the Lagrangian is a real local scalar functional, bilinear in Ψ in the sense that it can be presented in the form $F(R, S)R^2$, where $F(R, S)$ is a certain functional of R and S , their derivatives, and some external potential V .

The Hamiltonian operator can in principle be complex. As a matter of fact, this is the case even for the Hamiltonian of the ordinary Schrödinger equation. Indeed,

$$H_{SE}\Psi = \left[-\frac{\hbar^2 \Delta R}{2mR} + \frac{\hbar^2 (\vec{\nabla} S)^2}{2m} + \frac{i\hbar^2}{2mR^2} \vec{\nabla} \cdot (R^2 \vec{\nabla} S) + V \right] \Psi = H_{SE}(R, S)\Psi. \quad (2)$$

Usually, unlike in the linear case, the Hamiltonian operator of a modified equation is not Hermitian. It is sometimes required [13] that the operator in question be norm-Hermitian, i.e.,

$$\langle \Psi | H | \Psi \rangle \equiv \int d^3x \Psi^* (H\Psi) = \int d^3x (H\Psi)^* \Psi, \quad (3)$$

for any normalizable function Ψ in its domain. This ensures that the quantum-mechanical energy of a system, defined as the expectation value of its Hamiltonian H is real. As we will see, in some cases even real Lagrangian densities that entail a real field-theoretical energy lead to Hamiltonian operators that are not norm-Hermitian. Therefore, for the sake of the generality of our considerations, we do not insist that Hamiltonian operators discussed here possess this property. What we can observe on this example is that the Hamiltonian operator of a nonlinear modification of the Schrödinger equation is norm-Hermitian if

$$Im H_{NL}(R, S) = \frac{const}{R^2} \vec{\nabla} \cdot (f(R, S)), \quad (4)$$

where $f(R, S)$ is a certain functional of R and S that vanishes on the boundary. It should be pointed out that the Hamiltonian H_{SE} in its hydrodynamic nonlinear form (2) is not Hermitian, but, in fact, only norm-Hermitian. This an artifact of the nonlinear Madelung representation.

Knowing the Lagrangian $L(R, S)$ for a modification one derives the equations of motion for it in the hydrodynamic formulation by varying the Lagrangian with respect to R , S , and concomitant derivatives. Since for the linear Schrödinger equation

$$-L_{SE}(R, S) = \hbar R^2 \frac{\partial S}{\partial t} + \frac{\hbar^2}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + V R^2, \quad (5)$$

these equations have the form

$$\hbar \frac{\partial R^2}{\partial t} + \frac{\hbar^2}{m} \vec{\nabla} \cdot (R^2 \vec{\nabla} S) + \frac{\delta L_{NL}}{\delta S} = 0, \quad (6)$$

$$\frac{\hbar^2}{m} \Delta R - \frac{\hbar^2}{m} R (\vec{\nabla} S)^2 - 2\hbar R \frac{\partial S}{\partial t} - 2VR - \frac{\delta L_{NL}}{\delta R} = 0, \quad (7)$$

where $\delta L_{NL}/\delta S$ and $\delta L_{NL}/\delta R$ are Lagrangian derivatives with respect to S and R , correspondingly. If we write down the modified Schrödinger equation in the form resembling that of the linear equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi, \quad (8)$$

the imaginary part of it will lead to the continuity equation (6) and the real part to equation (7). Therefore,

$$H(R, S) = -\frac{\hbar^2 \Delta R}{2mR} + \frac{\hbar^2 (\vec{\nabla} S)^2}{2m} + V + \frac{1}{2R} \frac{\delta L_{NL}}{\delta R} + \frac{i\hbar^2}{2mR^2} \vec{\nabla} \cdot (R^2 \vec{\nabla} S) + \frac{i}{2R^2} \frac{\delta L_{NL}}{\delta S}, \quad (9)$$

from which we recognize that

$$H_{NL}(R, S) = \frac{1}{R} \frac{\delta L_{NL}}{\delta R} + \frac{i}{2R^2} \frac{\delta L_{NL}}{\delta S}. \quad (10)$$

The quantum-mechanical energy functional is

$$E_{QM} = \langle \Psi | H | \Psi \rangle = \int d^3x \left\{ \frac{\hbar^2}{2m} \left[R^2 (\vec{\nabla} S)^2 + (\vec{\nabla} R)^2 \right] + V R^2 + \frac{R}{2} \frac{\delta L_{NL}}{\delta R} + \frac{i}{2} \frac{\delta L_{NL}}{\delta S} \right\}, \quad (11)$$

where the term containing $\vec{\nabla} \cdot (R^2 \vec{\nabla} S)$ has not been included. Since it is a total derivative, when integrated over the entire space it produces zero owing to vanishing of R^2 on the boundary in the infinity. As already noted, this functional can be complex for the Hamiltonian operator is not necessarily norm-Hermitian.

The field-theoretical energy functional for the Lagrangian density that depends on R , S , and its first and second order derivatives stems from the following canonical energy-momentum tensor

$$T_\nu^\mu = \sum_i \left[\frac{\delta L}{\delta \partial_\mu \varphi_i} \partial_\nu \varphi_i + \frac{\delta L}{\delta \partial_\mu \partial_\alpha \varphi_i} \partial_\nu \partial_\alpha \varphi_i - \partial_\alpha \left(\frac{\delta L}{\delta \partial_\mu \partial_\alpha \varphi_i} \partial_\nu \varphi_i \right) - \delta_\nu^\mu L \right], \quad (12)$$

where $\varphi_i = (R, S)$, $i = 1, 2$. Defined as the space integral over the time-time component of this tensor, it reads

$$E_{FT} = \int d^3x \left\{ \frac{\hbar^2}{2m} \left[R^2 (\vec{\nabla} S)^2 + (\vec{\nabla} R)^2 \right] + V R^2 + L_{NL} \right\} + C, \quad (13)$$

where C is an arbitrary constant that can be put zero and which results from the integration of the conservation law

$$\partial_\mu T_\nu^\mu = 0. \quad (14)$$

We see that in general $E_{QM} \neq E_{FT}$. In particular, this holds true for the stationary states of a modified Schrödinger equation which are determined by the equation $\partial R^2 / \partial t = 0$. As long as $V \neq V(t)$, this equation together with (6-7) implies that, similarly as in the linear case, the stationary states have the form $\Psi = R \exp(-i\hbar\omega + \sigma(\vec{x}))$, where ω is the frequency. The energy of such states, E_ω , is by the virtue of the continuity equation real and equal $E_{QM} = \hbar\omega$, but even in such circumstances E_{QM} is not always equal to E_{FT} .

In its most general form suitable for our purposes, $L_{NL}(R, S)$ can be represented by $G(R, S)R^2$, where $G(R, S)$ is a functional of R , S , and their first and second order derivatives.² It can be shown that only if $G(R, S) = G_h(R, S)$, where G_h is homogeneous of degree zero in Ψ and such that

$$G_h(R, S) = \left[b_0 + b_1 \left(\frac{\vec{\nabla} R}{R} \right)^2 \right] p(S), \quad (15)$$

where

$$p(S) = a_1 (\vec{\nabla} S)^{2n_1} + a_2 (\Delta S)^{n_2} + a_3 (\vec{\nabla} S)^{2n_3} (\Delta S)^{n_4}, \quad (16)$$

²The expressions like $(\vec{\nabla} S \times \vec{\nabla} S)^2$, $(\vec{\nabla} S \times \vec{\nabla} R)^2 / R^2$ or $(\vec{\nabla} R \times \vec{\nabla} R)^2 / R^4$ are excluded from our considerations. In general, they would entail the ambiguity.

and a_i, b_i are real constants and n_i non-negative integers, the ambiguity in question disappears, i.e.,

$$E_{QM} = E_{FT} = \int d^3x \left\{ \frac{\hbar^2}{2m} \left[R^2 (\vec{\nabla} S)^2 + (\vec{\nabla} R)^2 \right] + V R^2 + G_h(R, S) R^2 \right\}, \quad (17)$$

with $C = 0$. We will denote the Lagrangian of this property by $L_h(R, S)$. The discussed homogeneity of $G_h(R, S)$ implies in particular that G_h cannot be polynomial in S , but needs to depend on S through at least first order derivatives. Indeed, since $S = \frac{i}{2} \ln(\Psi/\Psi^*)$, $S(\lambda\Psi, (\lambda\Psi)^*) \neq S(\Psi, \Psi^*)$ and one can easily show that if G is proportional to S^k , $E_{QM} \neq E_{FT}$. This demonstration and the proof that $G_h(R, S)$ has to be of the form (15-16) are relegated to the appendix. This constitutes the main result of the present paper.

3 Examples

In what follows, we will adopt the convention $\hbar = 1$. To begin with, let us consider a simple nonhomogenous model Lagrangian density that in its inhomogenous part employs terms similar to those in the Lagrangian density for the linear Schrödinger equation. The nonlinear part of the Lagrangian density for the modification is

$$L_{NL} = a (\vec{\nabla} S)^2 + b \left(\frac{\vec{\nabla} R}{R} \right)^2, \quad (18)$$

where a and b are certain dimensional constants. The equations of motion read

$$\frac{\partial R^2}{\partial t} + \vec{\nabla} \cdot (R^2 \vec{\nabla} S) + 2a \Delta S = 0, \quad (19)$$

$$\frac{1}{m} \Delta R + 2b \left[\frac{1}{R} \left(\frac{\vec{\nabla} R}{R} \right)^2 + \vec{\nabla} \cdot \left(\frac{\vec{\nabla} R}{R^2} \right) \right] - \frac{1}{m} R (\vec{\nabla} S)^2 - 2R \frac{\partial S}{\partial t} - 2VR = 0. \quad (20)$$

From these the nonlinear part of the Hamiltonian is identified with

$$H_{NL} = -i \frac{a \Delta S}{R^2} + b \frac{\Delta \ln R^2}{R^2}. \quad (21)$$

The quantum-mechanical energy of a system described by R and S is then

$$E_{QM} = \int d^3x \left\{ \frac{1}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + V R^2 + b \Delta \ln R^2 - i a \Delta S \right\}. \quad (22)$$

However, one finds that the field-theoretical energy functional for this case is

$$E_{FT} = \int d^3x \left\{ \frac{1}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + V R^2 + a (\vec{\nabla} S)^2 + b \left(\frac{\vec{\nabla} R}{R} \right)^2 \right\}. \quad (23)$$

To convince ourselves that these two expressions for the energy give different results let us set³ $b = 0$ and consider the case of a one-dimensional coherent state wave packet. Such a packet requires the

³This model of NLSE should not be construed as anything else than a toy model intended solely for the purpose of this exposition. To make it less toyish one should put $b = 0$ anyway so as to allow a greater class of physically acceptable solutions which for an arbitrary $b \neq 0$ would be excluded by the condition of finite energy.

potential of a simple harmonic oscillator, $V = m\omega^2 x^2/2$. Its amplitude and phase are given by ($x_0 = 1/\sqrt{m\omega}$.)

$$R_{coh}^2 = \frac{1}{\sqrt{\pi}x_0} \exp \left[-\frac{(x - x_0\sqrt{2}\cos(\omega t - \delta))^2}{x_0^2} \right] \quad (24)$$

and

$$S_{coh} = -\left(\frac{\omega t}{2} - \frac{|\alpha|^2}{2} \sin 2(\omega t - \delta) + \frac{\sqrt{2}|\alpha|x}{x_0} \sin(\omega t - \delta) \right), \quad (25)$$

correspondingly, where α and δ are arbitrary numbers, complex and real, respectively. The coherent state is a solution to our equations of motion as its phase satisfies $\Delta S_{coh} = 0$. Now, since $\vec{\nabla} S_{coh}$ is not identically zero, the expressions in question produce completely different values for the energy of this state. In fact, E_{FT} is infinite for most of the time! One might think that this modification is too contrived. However, a similar situation occurs in the Staruszkiewicz modification of the Schrödinger equation [41] which can be derived from the Lagrangian

$$-L_{SM} = R^2 \frac{\partial S}{\partial t} + \frac{1}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + R^2 V + \frac{c}{2} (\Delta S)^2 \quad (26)$$

leading to the equations

$$\frac{\partial R^2}{\partial t} + \frac{1}{m} \vec{\nabla} \cdot (R^2 \vec{\nabla} S) - c \Delta \Delta S = 0, \quad (27)$$

$$\frac{1}{m} \Delta R - R (\vec{\nabla} S)^2 - 2R \frac{\partial S}{\partial t} - 2VR = 0. \quad (28)$$

The field-theoretical form of the energy functional for this modification,

$$E_{FT} = \int d^3x \left\{ \frac{1}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + \frac{c}{2} (\Delta S)^2 + VR^2 \right\}, \quad (29)$$

is again different from its quantum-mechanical counterpart,

$$E_{QM} = \int d^3x \left\{ \frac{1}{2m} \left[(\vec{\nabla} R)^2 + R^2 (\vec{\nabla} S)^2 \right] + VR^2 + \frac{ic}{2} \Delta \Delta S \right\}, \quad (30)$$

which can be easily obtained from the Hamiltonian for this modification

$$H_{SM} = H_{SE} + \frac{ic\Delta\Delta S}{2R^2}. \quad (31)$$

Now, even if these two energy functionals are equal for the coherent state they do drastically differ for ordinary Gaussian wave packets for which $\Delta S = g(t)$. Obviously, these wave packets are solutions to the equations of motion of the modification.

The energy functionals E_{QM} discussed so far contain imaginary components. Since the energy is supposed to be a real quantity one might want to require that these parts do not contribute to the total energy, which imposes a constraint on physically acceptable states allowed by these particular nonlinear models of the Schrödinger equation. That these constraints are not necessarily very restrictive or physically unjustified can be seen from the Staruszkiewicz modification for which E_{FT} is infinite for Gaussian wave packets which therefore should be excluded if this energy definition were employed and which are perfectly fine on the energetic grounds if one uses the quantum-mechanical definition

of energy. Moreover, the continuity equation implies vanishing of the imaginary terms for a large class of physically interesting situations. The condition of real energy in the cases presented (if one assumes a less restricting case of $b = 0$ in the toy model described by (19) and (20)) is equivalent to the selection of observables in NLQM, or, more precisely, of their domain, for which contributions of nonlinear parts vanish on normalized states. This in itself does not resolve the problem of ambiguity as even if E_{QM} is now real it is still in general different from E_{FT} . What it does though is to illustrate the fact that the properties of observables depend on the space of states on which they are defined. This is so in particular in linear QM, where, for instance, the self-adjointness of an operator depends on its domain. It is in line with this observation that one can attempt to reconcile E_{QM} with E_{FT} by choosing a domain in which they are equal for each function in this domain. Nevertheless such an alternative would be overly restrictive in some cases, to the extent that it would result in a trivial and physically unsatisfactory domain. The simplest example of the modification of this kind is provided by the well-known nonlinear cubic Schrödinger equation for which $L_{NL} = R^4$. One could also completely reject the statistical definition of energy in quantum theory, E_{QM} , but this would constitute a very dramatic departure from the conceptual structure of this theory. In fact, by identifying the class of modifications for which $E_{QM} = E_{FT}$, we demonstrated that this is not necessary.

We have limited our considerations to local Lagrangian densities, but it can be shown that the ambiguity in question occurs also in modifications that stem from nonlocal nonhomogeneous Lagrangians. For some particular form of the nonlinear part of the Lagrangian density,

$$L'_{NL} = G(\rho)\rho = \int_0^\rho d\rho' F(\rho'), \quad (32)$$

this has been demonstrated in [12]. This Lagrangian leads to the Hamiltonian $H'_{NL} = F(\rho)$, where F is a functional of $\rho = R^2$ and it is assumed that it contains no derivatives. One has

$$E_{QM} - E_{FT} = \langle \Psi | F | \Psi \rangle - \langle \Psi | G | \Psi \rangle - C = D - C. \quad (33)$$

The discussed class of nonhomogeneous modifications includes as a special case the Białynicki-Birula and Mycielski modification [12] characterized by $F(\rho) = c_1 \ln c_2 \rho$, where c_1 and c_2 are constants. This modification is an exception to the rule as here $D = c_1$ for wave functions normalized to unity and so by choosing $c_1 = C$ one causes the ambiguity to disappear. The Białynicki-Birula and Mycielski modification can in fact be thought of as a homogeneous modification modulo the phase gauge transformation $S \rightarrow S - 2i \ln |\lambda|$ which when exercised along with the homogeneity transformation $\Psi \rightarrow \lambda \Psi$ renders the NLSE of the modification homogeneous. It is also this gauge transformation that removes the difference between E_{QM} and E_{FT} . Moreover, as shown in [12], if $E_{QM} = E_{FT}$ for all stationary states of $H = H_{SE} + H'_{NL}$ then the nonlinearity must be logarithmic as in the modification under consideration, which proves the generic nature of the ambiguity in the class of nonlinear modifications derivable from the nonlocal Lagrangian (32).

Let us now discuss the examples of modifications known in the literature that derive from local Lagrangian densities in which the ambiguity problem does not arise. The first of them constitutes a restricted version of the Doebner-Goldin modification [32, 33] for which the Lagrangian density was found in [37]. The density in question reads

$$L_{DG}^r(R, S) = L_{SE} + c_1 R^2 \Delta S. \quad (34)$$

Its nonlinear part is clearly a special version of $L_h(R, S)$ for which b_1 in (15), a_1 and a_3 in (16) are zero, and n_2 in (16) is 1. A more general Lagrangian that encompasses L_{DG}^r as a special case was

introduced in [37]. It is given by

$$L_{PH}(R, S) = L_{SE} + c_1 R^2 (\Delta S)^n \quad (35)$$

and corresponds to special but fairly general a Galilean invariant version of our $L_h(R, S)$ with $b_1 = a_1 = a_3 = 0$ in (15-16) and an arbitrary $n_2 = n$ in (16). The particular case of $n = 2$ was treated in more detail in [37, 42]. It should be noted that a generalization of $p(S)$ of (16) is still possible; the terms $(\Delta^m S)^n$, where $m > 1$, and their products with $(\vec{\nabla} S)^{2k}$ can be added to $p(S)$ without violating the equivalence of E_{QM} and E_{FT} . The latter case represents the most general scheme proposed in [37].

4 Conclusions

We have noted and discussed the ambiguity in the definition of the energy functional in NLQM. As opposed to linear theory, the energy functional defined as the expectation value of the Hamiltonian operator is not equal to the conserved quantity derived within the Lagrangian field-theoretical framework that one identifies with the energy of a system. It has been shown that inspite of the generic nature of this ambiguity, there exists a class of nonlinear modifications of the Schrödinger equation derivable from local Lagrangian densities in which the ambiguity in question does not arise. This is tantamount to the definition of a new class of such modifications uniquely characterized by the property in question. The modifications of this class must be homogeneous in the wave function and, as a rule, they involve spatial derivatives of its phase in their NLSE. It is the presence of the phase functionals in the Lagrangian densities that is the most salient feature of this class. Paradoxically enough, the phase modifications of the Schrödinger equation have not been particularly pursued in the literature. Only two examples of the class under consideration have been proposed so far [33, 37], although their exceptionality in the sense discussed have not been fully realized.

We see therefore that even if the homogeneity of NLSE is neither necessary for its strong [21] nor sufficient for its weak separability [37], preserving this property in the NLSE certainly adds to the congruency of the formulation of NLQM and warrants that one of highly desirable features of linear theory, the non-ambiguous definition of energy, does not have to be abandoned, but can be retained this special scheme of modifications. It also makes this type of modifications more similar to the linear SE, and saves us from resorting to more radical means of resolving this problem as, for instance, rejecting the statistical interpretation of quantum theory and, consequently, E_{QM} as a viable definition of energy. As found in [37] for some Galilean invariant subclass of this scheme, the modifications in question do not have the standard Ehrenfest limit, which suggests that they are not linearizable and thus can describe some new physics that the linear theory is unable to capture. Further studies are necessary to understand all the physical implications of this unique property that defines the discussed class of modifications.

Let us note that despite the fact that the nonlinear Hamiltonians we considered are manifestly non-Hermitian, their expectation values are real numbers. Although relatively little known, this also happens to be true for linear operators [43], and, quite recently, it has been observed for some surprisingly simple complex-valued one-dimensional potentials [44]. The Hermiticity of Hamiltonians is sometimes also purposely sacrificed in linear QM in order to simplify description of complex phenomena involving many degrees of freedom not all of which can be taken into account. For instance, it is well known that to describe absorption in scattering processes, such as elastic scattering

in nuclear physics, one can implement complex or “optical” potentials. Such potentials can also be used to describe decoherence [45]. It should also be noted that not all equations of physical interest can be derived from local Lagrangian densities; the best case in point is provided by the celebrated Navier-Stokes equations for which no Lagrangian exists [46].

In the course of this work, we became aware that the discussed energy ambiguity was observed by other authors as well. We have already alluded to this when discussing the modifications that stem from nonlocal Lagrangian densities. The special case of such modifications was discussed by Białynicki-Birula and Mycielski [12] mainly as a way to emphasize the uniqueness of their model. Some more attention this issue received in the work of Shapiro [47]. Both papers considered only real nonlinear Lagrangian corrections and none of them examined general conditions under which $E_{QM} = E_{FT}$. Neither did they point out the relevance of the homogeneity as an important prerequisite for the equivalence of the energy functionals in question.

5 Appendix

We will demonstrate here that the most general form of $G(R, S)$ that satisfies our conditions and ensures that $E_{QM} = E_{FT}$ is of the form (15-16). The general nonhomogeneous form of $G(R, S)$ is

$$G(R, S) = G_h(R, S) \left[\sum_{k=1} S^k + \sum_{l=1} R^l + \sum_{m,n=1} S^m R^n \right],$$

where the homogeneous part can be presented as

$$G_h(R, S) = p(S) + q(R) + t(R, S),$$

with

$$\begin{aligned} p(S) &= a_1 (\vec{\nabla} S)^{2n_1} + a_2 (\Delta S)^{n_2} + a_3 (\vec{\nabla} S)^{2n_3} (\Delta S)^{n_4}, \\ q(R) &= b_1 \left(\frac{\vec{\nabla} R}{R} \right)^{2k_1} + b_2 \left(\frac{\Delta R}{R} \right)^{k_2} + b_3 \left(\frac{\vec{\nabla} R}{R} \right)^{2k_3} \left(\frac{\Delta R}{R} \right)^{k_4}, \\ t(R, S) &= cp(S)q(R), \end{aligned}$$

and where a_i, b_i, c are some constants. The exponents m and n are in general different from the ones used below in some particular cases. For the sake of completeness, let us recall that

$$E_{QM} = \int d^3x \left\{ \frac{\hbar^2}{2m} \left[R^2 (\vec{\nabla} S)^2 + (\vec{\nabla} R)^2 \right] + V R^2 + \frac{R}{2} \frac{\delta L_{NL}}{\delta R} + \frac{i}{2} \frac{\delta L_{NL}}{\delta S} \right\}$$

and

$$E_{FT} = \int d^3x \left\{ \frac{\hbar^2}{2m} \left[R^2 (\vec{\nabla} S)^2 + (\vec{\nabla} R)^2 \right] + V R^2 + L_{NL} \right\}.$$

To begin with, let us first discuss the case of $q_1(R) = b_1 (\vec{\nabla} R/R)^{2m} R^2$. One obtains that

$$\frac{R}{2} \frac{\delta q_1(R)}{\delta R} = \frac{(1-2m)b_1}{2} \left(\frac{\vec{\nabla} R}{R} \right)^{2m-2} R^2 \left[(2-2m) \left(\frac{\vec{\nabla} R}{R} \right)^2 + 2m \left(\frac{\Delta R}{R} \right) \right]$$

and consequently, since $\int d^3x R \Delta R = -\int d^3x (\vec{\nabla} R)^2$, it is only for $m = 1$ that $E_{QM}[q_1(R)] = E_{FT}[q_1(R)]$. For $q_2(R) = b_2 (\Delta R/R)^n R^2$ we derive that

$$\begin{aligned} \frac{R \delta q_2(R)}{2 \delta R} &= \frac{b_2 R^2}{2} \left\{ A_2(R) \left(\frac{\Delta R}{R} \right)^n + \right. \\ &\quad \left. n \left[B_2(R) \left(\frac{\Delta R}{R} \right)^{n-1} + C_2(R) \left(\frac{\Delta R}{R} \right)^{n-2} + D_2(R) \left(\frac{\Delta R}{R} \right)^{n-3} \right] \right\} \end{aligned}$$

where

$$\begin{aligned} A_2(R) &= (2-n)(1+n), \\ B_2(R) &= (2-n)(1-n) \left(\frac{\vec{\nabla} R}{R} \right)^2, \\ C_2(R) &= (n-1) \left[\frac{\Delta^2 R}{R} + 2(2-n) \frac{\vec{\nabla} R}{R} \cdot \frac{\vec{\nabla} \Delta R}{R} \right], \\ D_2(R) &= (n-1)(n-2) \left(\frac{\vec{\nabla} \Delta R}{R} \right)^2. \end{aligned}$$

One can see that under no circumstances $E_{QM}[q_2(R)] = E_{FT}[q_2(R)]$. We expect thus that the same happens for $q_3(R) = b_3 (\vec{\nabla} R/R)^{2m} (\Delta R/R)^n R^2$. This is indeed the case as

$$\begin{aligned} \frac{R \delta q_3(R)}{2 \delta R} &= \frac{b_3}{2} \left(\frac{\vec{\nabla} R}{R} \right)^{2m-2} R^2 \left\{ A_3(R) \left(\frac{\Delta R}{R} \right)^n + \right. \\ &\quad \left. n \left[B_3(R) \left(\frac{\Delta R}{R} \right)^{n-1} + C_3(R) \left(\frac{\Delta R}{R} \right)^{n-2} + D_3(R) \left(\frac{\Delta R}{R} \right)^{n-3} \right] \right\}, \end{aligned}$$

where

$$\begin{aligned} A_3(R) &= \alpha [1 - 2m + n(1 + 4m)] \left(\frac{\vec{\nabla} R}{R} \right)^2 - 2m(1 - 2m)(n-1) \frac{\Delta R}{R}, \\ B_3(R) &= \alpha(\alpha - 1) \left(\frac{\vec{\nabla} R}{R} \right)^4 + 2m(2n - 3) \frac{\vec{\nabla} R}{R} \cdot \frac{\vec{\nabla} \Delta R}{R}, \\ C_3(R) &= (n-1) \left[\frac{\Delta^2 R}{R} + 2\alpha \frac{\vec{\nabla} R}{R} \cdot \frac{\vec{\nabla} \Delta R}{R} \right] \left(\frac{\vec{\nabla} R}{R} \right)^2, \\ D_3(R) &= (n-1)(n-2) \left(\frac{\vec{\nabla} \Delta R}{R} \right)^2 \left(\frac{\vec{\nabla} R}{R} \right)^2, \end{aligned}$$

and $\alpha = 2 - 2m - n$. For these reasons it is only $t(R, S) = cp(S)q_1(R)$ that can guarantee that $E_{QM}[t(R, S)] = E_{FT}[t(R, S)]$. To see why it is so and why $p(S)q_2(R)$ would not work let us consider an example that also proves that $p(S)R^2$ does not lead to the ambiguity in question. Let us take

$$L_{NL}^* = p(S) \left[R^2 + b_1 (\vec{\nabla} R)^2 + b_2 (\Delta R)^2 \right] = p(S)q^*(R).$$

Now,

$$\frac{\delta L_{NL}^*}{\delta S} = -\vec{\nabla} \cdot \left[\frac{\partial p(S)}{\partial \vec{\nabla} S} q^*(R) \right] + \Delta \left[\frac{\partial p(S)}{\partial \Delta S} q^*(R) \right]$$

which as a total derivative of R and its concomitants does not contribute to the quantum-mechanical energy functional. We also have

$$\frac{R}{2} \frac{\delta L_{NL}^*}{\delta R} = p(S)R^2 - b_1 R \vec{\nabla} \cdot (p(S) \vec{\nabla} R) + b_2 R \Delta (p(S) \Delta R)$$

and since $R \vec{\nabla} \cdot (p(S) \vec{\nabla} R) = \vec{\nabla} \cdot (p(S) R \vec{\nabla} R) - p(S) (\vec{\nabla} R)^2$, $\int d^3x R \vec{\nabla} \cdot (p(S) \vec{\nabla} R) = -\int d^3x p(S) (\vec{\nabla} R)^2$. Because of that, one can have $E_{QM}[L_{NL}^*] = E_{FT}[L_{NL}^*]$, but only if $b_2 = 0$.

We will now consider the general case. It is easy to understand why the general nonhomogeneous form of $G(R, S)$ would generate the energy ambiguity even if $G_h(R, S)$ is chosen in such a way that it does not cause it itself. Let us put m and n in the expression for $G(R, S)$ equal zero and treat first the case $l = 0$. One notes that $\delta[G(R, S)R^2]/\delta S$ contains terms proportional to S^{k-1} that are not total derivatives. As a result, E_{QM} is complex as opposed to E_{FT} which is always real. On the other hand, even if $k = 0$, the absence of the ambiguity requires that

$$\int d^3x R \frac{\delta[G(R, S)R^2]}{2\delta R} = \int d^3x G(R, S)R^2,$$

which happens only if $l = 0$. We see now that the case of $m \neq 0$ and $n \neq 0$ only compounds the problem.

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